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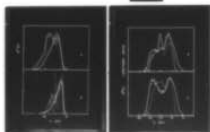
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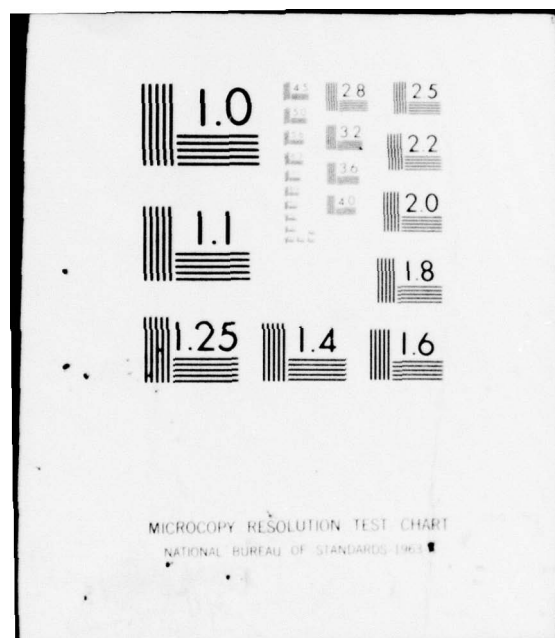
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TRANSITION DENSITY OF STATES FOR Si(100) FROM
 $L_1L_{23}V$ and $L_{23}VV$ AUGER SPECTRA

by

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Transition Density of States for Si (100)
from $L_1L_{23}V$ and $L_{23}VV$ Auger Spectra*

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ABSTRACT

The $L_1L_{23}V$ and $L_{23}VV$ Auger spectra of sputtered and annealed Si(100) have been measured and the transition density of states extracted. The line shapes for the two transitions differ, indicating the importance of matrix element effects. Whereas the $L_1L_{23}V$ line shape closely resembles results of other measurements of the Si density of states, the $L_{23}VV$ line shows a strong emphasis on p-like states.

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INTRODUCTION

Auger electron spectroscopy (AES), in addition to being a rapid, experimentally simple method of surface elemental analysis, is a probe of the valence-band states in any transition for which these states are involved, and thus should in principle contain a considerable amount of surface chemical bonding information. Because it is a two-electron spectroscopy, however, AES has been considered much harder to interpret than other valence-band-sensitive spectroscopies, such as photoelectron spectroscopy (PES), that have similar surface sensitivity. However, it is precisely the two-electron nature of AES that makes it an attractive and distinctly different tool for the study of surface electronic properties, by permitting a view of the local density of states (DOS) from different ion cores in compounds or substrate-adsorbate systems. Furthermore, the Auger process provides an additional way of looking at the relaxation shifts inherent in all electron spectroscopies. Finally, an understanding of Auger lineshapes is required to make AES a quantitative surface analytical tool.

The matrix element for the Auger transition⁽¹⁾ involves the Coulomb potential, connecting final states represented by a core wave function and an appropriate continuum wave function (identical in form to a low-energy-electron-diffraction wave function) with initial states represented respectively for core-valence-valence (CVV) or core-core-valence (CCV) transitions by two valence-electron wave functions or a core-electron and a valence-electron wave function. It is easy to show by expanding the potential in terms of the vector separation of ion cores, \vec{R} , that the Auger matrix element $M \propto \frac{1}{R^3}$ and that there-

fore the probability of interatomic Auger processes falls off very rapidly with the separation of the cores.⁽²⁾ Hence the Auger current is characteristic of a local density of filled states at the atom on which the original core hole was made. This picture is in contrast to photoelectron spectroscopy (PES), where a non-local DOS, including interference effects over many lattice constants, is measured.

For any electron spectroscopy, the line shape is distorted by transition probability variations across the measured spectrum and by extraatomic relaxation effects. The former have been generally assumed constant for Auger processes.⁽³⁾ Because AES involves two final-state holes, the latter have been assumed to be severe,⁽⁴⁻⁶⁾ and in fact, there is evidence that in some systems it is not possible to extract reliable DOS information from Auger data.

We have measured and compared the $L_{23}VV$ and $L_1L_{23}V$ Auger spectra from sputtered and annealed Si(100). We demonstrate that relaxation effects do not have a major effect on the line shape. On the other hand, there is clear evidence that transition probability effects are important.

An n-doped 10 Ω -cm Si(100) wafer was sputtered for sufficient time to remove all impurities except for a trace of C. Measurements on the resulting surface were made with a single-pass cylindrical mirror analyzer at a resolution of ~ 1.2 eV, and the data averaged on a Nicolet 1074 signal averager. The crystal was then annealed for 15 min at 1200°C. The energy loss spectrum after annealing was identical to that reported for annealed Si(100).⁽⁷⁾ Independent LEED measurements with the same sputtering and annealing conditions showed only a diffuse background for the sputtered sample and a sharp diffraction pattern for the annealed surface. We take these results as evidence of a rea-

sonably well-ordered Si(100) surface for the annealed sample and an essentially amorphous layer for the sputtered sample. The Auger data were integrated and deconvoluted with an instrument/loss function approximated by the electron backscatter spectrum at the energy of the Auger feature.⁽⁸⁾ The resulting Auger line shapes $N^*(E)$ are shown in Figures 1 and 2 as solid curves.

The main feature of the dN/dE Auger spectrum of any Si surface is the L_{23}^{VV} line at 91 eV. It has been shown that the differences in this line for cleaved Si(111)(2×1) and annealed Si(111)(7×7) are quite small.⁽⁹⁾ The same is true for sputtered and annealed Si(100), with only a small bump appearing at ~ 83 eV for the annealed surface that manifests itself as a weak shoulder in the $N^*(E)$ spectrum.⁽¹⁰⁾

The simplest view of an LVV transition is that it represents a self-convolution of the valence-band density of states.^(11,12) This cannot be strictly correct, since the Auger line shape consists of some average of densities of states that can differ from layer to layer near the surface, and also since transition probability variations may occur across the band even for a density of states independent of depth below the surface. In Figure 1a, our Auger data are compared to the self-convolution of both the crystalline⁽¹³⁾ and amorphous⁽¹⁴⁾ theoretical densities of states. Several features are immediately obvious:

(1) The self-convolutions of the amorphous and crystalline calculations are quite similar, differing only in detail in the s-like states. Hence, even for the best possible case, one could not expect to see significant

differences in an LVV Auger line shape for amorphous and crystalline Si. (2) The measurement greatly emphasizes the upper, p-like states⁽¹⁵⁾ with respect to the s states. Without detailed analysis, one can state that transition probability effects are important in this transition. This is borne out by detailed one-electron calculations of the LVV Auger line shape for an unreconstructed Si(111) surface, which show that the contributions from the p-like matrix elements are dominant.⁽¹⁶⁾ (3) The line width is quite similar to theory,^(13,14,16b) indicating that differential relaxation across the band does not have a significant effect for this line. Screening of the initial L_{23} core hole can cause differential relaxation of atomic orbitals; however, in Si, this amounts to only ~ 1 eV for the 3s and 3p levels.⁽¹⁷⁾

Final-state relaxation can be due either to hole-hole interactions or polarization effects; their sum may have either sign, depending on which dominates. Since no significant broadening is observed, we conclude that these effects are not important here. However, the large dominance of the p-like matrix elements may make questions of differential relaxation for the LVV line less significant.

The absolute energy position of the LVV line is within contact potential differences of that calculated using XPS electron binding energies.

To facilitate comparison with the $L_1L_{23}V$ Auger transition, Figure 1b shows the convolution square root of the $L_{23}VV$ data; it indicates again the emphasis on p states relative to calculations for bulk crystalline⁽¹³⁾ and amorphous⁽¹⁴⁾ theoretical densities of states. However, the fit is much better, especially for the amorphous case; because of its properties, the convolution in Figure 1a tends to magnify the differences in the curves in Figure 1b.

Direct evidence for matrix element effects comes by comparing Figure 1b with the $L_1L_{23}V$ line, shown in Figure 2, which gives the transition density of states directly.^(18,19) Figure 2a shows the $L_1L_{23}V$ line shape for annealed Si(100) compared to photoelectron spectroscopy results.^(20,21) The Auger line has been deconvoluted with a Lorentzian of 1.75 eV FWHM, which represents an estimate of the upper limit of the inverse lifetime of this transition.⁽²²⁾ Several points can be made: (1) The structure in the Auger line corresponds well in position with other measurements and theory, and reasonably well in the relative amplitudes of the structure. (2) The structure is less well resolved (e.g., the central, sharp peak is reduced in amplitude); both lifetime broadening and the limited detector resolution contribute to this. (3) The total line width is somewhat too broad compared to other measurements. This can be attributed almost totally to tailing of the edges of the line, especially the leading edge, which rises slowly relative to other results. This may be an artifact of the data reduction. It could, of course, be attributed to differential relaxation across the band, but the fact that the peaks are not shifted relative to PES results argues against this view. (4) The line width is the same as in Figure 1b, but the s states have considerably more intensity. Whereas the $L_1L_{23}V$ line appears to have a relatively constant transition probability across the band (at least compared to other measurements), the $L_{23}VV$ line clearly has strong matrix element effects.

The absolute energy position of the $L_1L_{23}V$ line is 2.5eV lower than that calculated using XPS binding energies. This value is determined using the first peak in the line rather than the zero crossing of the leading edge.

Figure 2b shows, finally, the $L_1L_{23}V$ line for sputtered Si(100). Whereas the upper p -like states are unaffected, the sharp central s-p-like peak disappears, in agreement with theory. In addition, however, the lower s -like states become very strong, in disagreement with bulk theory, but in agreement with results on Si surfaces with high step densities.⁽²³⁾ We suggest that this large peak is a surface effect, caused by the increase in the number of backbonding states created when the surface is damaged and the average coordination number of a surface atom is reduced.

We have made similar measurements on Si(111). A comparison shows a number of other features that may be interpreted in terms of surface effects.⁽²⁴⁾ In summary, we have extracted transition DOS's for Si(100) from both the $L_1L_{23}V$ and $L_{23}VV$ Auger lines. Differential relaxation effects do not seem to be important, and whereas the $L_1L_{23}V$ line reproduces the DOS reasonably well, strong emphasis on p-like states in the $L_{23}VV$ line distort that line shape considerably.⁽²⁵⁾ As in photoelectron spectroscopy, it is possible to extract a transition density of states, but it does not appear to be possible to interpret these a priori in terms of the actual density of states without a detailed knowledge of the matrix elements involved.

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FIGURE CAPTIONS

Fig. 1 Comparison of L_{23}^{VV} Auger line shape for Si(100) with theory. a) Solid curve: present results. Dotted curve: self-convolution of crystalline Si DOS, Ref. 13. Dashed curve: self-convolution of amorphous Si DOS, Ref. 14. b) Solid curve: Convolution square root of present results. Dotted curve: crystalline Si DOS. Dashed curve: amorphous Si DOS.

Fig. 2 Comparison of $L_1L_{23}^V$ Auger line shape for Si(100) with other measurements. a) Annealed Si(100). Solid curve: present results. Dotted curve: ultraviolet photoemission from Si(100) Ref. 21. Dashed curve: x-ray photoemission from cleaved Si, Ref. 20. b) Sputtered Si(100). Solid curve: present results. Dashed curve: x-ray photoemission from amorphous Si, Ref. 20.

$N^*(E)$

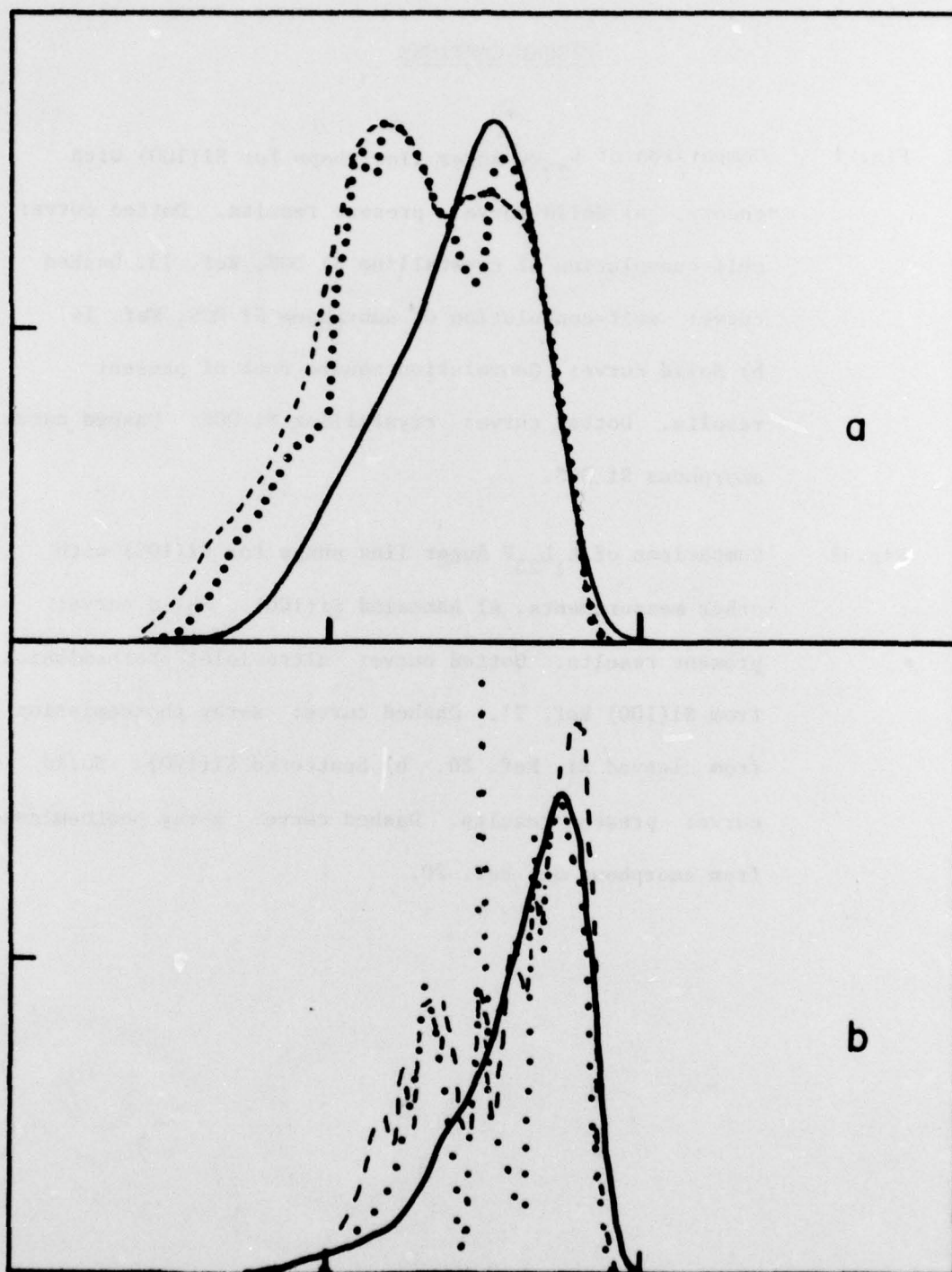
a

b

-16

0

E (eV)



$N^*(E)$ (ARBITRARY UNITS)

$N^*(E)$

